# 3rd RSC/SCI Symposium on GPCRs in Medicinal Chemistry

Monday 20 - Wednesday 22 September 2010

MSD, Oss, The Netherlands

RSC | Advancing the Chemical Sciences

**Organised by SCI's Fine Chemicals Group and RSC's Biological & Medicinal Chemistry Sector**

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Programme

## Monday 20 September

**09:00** Registration and refreshments

**09:45** **Welcome**
Caroline Low, Imperial College, UK

Session 1 Structural Influences on Lead Generation

**10:00** **Plenary: The crystal structure of the adenosine A2A receptor - implications for GPCR drug design**
Ad IJzerman, Medicinal Chemistry, Leiden, The Netherlands

**10:45** **The discovery of Lu AA47070 - An A2A receptor antagonist prodrug**
Anette Graven Sams, Lundbeck Research, Denmark

**11:30** Refreshments

**12:00** **Elucidation of the binding mode of anticholinergics in the M3 receptor by mutagenesis experiments and molecular modeling**
Christofer Tautermann, Boehringer Ingelheim Pharma, Germany

**12:45** **Novel histamine GPCR family antagonists by fragment screening and molecular modeling**
Richard J Law, Evotec, UK

**13:30** Lunch

Session 2 GPCR Class A Ligands

**14:30** **De novo design of a picomolar non-basic 5-$HT_{IB}$ receptor antagonist**
Peter Bernstein, AstraZeneca, USA

**15:15** **Discovery of lorcaserin: A selective 5-$HT_{2C}$ receptor agonist for the treatment of obesity**
Brian Smith, Arena Pharmaceuticals, USA

**16:00** Refreshments

**16:30** **Sitting on a goldmine: Knowledge based design of 5-HT2b antagonists**
David Hirst, GlaxoSmithKline, UK

**17:15** **Discovery of novel and orally available GPR40 agonists for the treatment of type 2 diabetes**
Tsuneo Yasuma, Takeda Pharmaceutical Company, Japan

**18:00** Posters and wine reception

Free evening in Oss

## Tuesday 21 September

Session 1 7TM Peptide Receptors

**09:00** **The discovery of GSK962040; the first small molecule motilin receptor agonist clinical candidate**
Sue Westaway, GlaxoSmithKline, UK

**09:45** **Low molecular weight gonadotrophins - fertile grounds in drug discovery**
Brigitte Folmer, MSD, The Netherlands

**10:30** Refreshments

**11:00** **Once daily B2 agonists for the management of asthma and COPD: molecular rationale for the long duration of action**
Paola Casarosa, Boehringer Ingelheim Pharma, Germany

**11:45** **Close to the edge: Optimisation of a series of neutral MC4 agonists**
Mark Andrews, Pfizer, UK

**12:30** Lunch

Session 2 Allosteric Modulators

**14:00** **Plenary: Allosteric modulation of GPCRs: Discovery and development of selective mAchR allosteric ligands**
Carrie K. Jones, Vanderbilt, USA

**14:45** **Allosteric antagonists of CCR4**
David Cheshire, AstraZeneca, UK

**15:30** Refreshments

**16:00** **Discovery of novel orally active mGluR5 antagonist GSK2210875**
Steve Watson, GSK Neurosciences CEDD, UK

**16:45** **Positive allosteric modulation of the mGlu2 receptor in the treatment of CNS disorder**
Gregor MacDonald, Johnson and Johnson, Belgium

**17:30** **Hit to lead chemistry in two GPCR targets for tackling pain**
Dafydd Owen, Pfizer, UK

**19:30** Gala Dinner@MSD

## Wednesday 22 September

Session 1 7TMs: New Technologies in GPCR Research

**09:00** **G protein-independent assays for screening of seven transmembrane receptors**
Miranda van der Lee, MSD, Merck Research Laboratories, The Netherlands

**09:45** **GPCR allosteric modulator discovery: Silence is golden**
Stephan Schann, Domain Therapeutics

**10:30** Refreshments

**11:00** **Use of stabilised receptors for fragment screening & SBDD**
Malcolm Weir, Heptares Therapeutics, UK

**11:45** **Outside the cytoplasm, biophysical ligand screening for membrane proteins?**
Gregg Siegal, Univ.Leiden / Zobio, The Netherlands

**12:30** Close

## Synopsis

G-protein coupled receptors play a crucial role in transmitting chemical signals from hormones and nerotransmitters across cell membranes and converting them into cellular responses.

G-protein coupled receptors drive processes as diverse as cell development and proliferation, neuromodulation, metabolic disorders, inflammation, and viral infection. As such, these receptors are involved in many diseases and continue to represent the target of a large proportion of all modern medicinal drugs. This years symposium will highlight two particular themes: the impact of recent breakthroughs in X-ray structure determination on GPCR drug discovery; and allosteric regulation of GPCR activity. Presentations will also include a wide range of medicinal chemistry case histories, real examples of drug discovery in practise from the bench to the clinic.

*Supported by* MSD

## Exhibition & Posters

There will be a limited number of spaces available for organisations who may wish to exhibit. For further information please send an email to conferences@soci.org. If you would like to present a poster, applicants should submit an A4 abstract to conferences@soci.org. The deadline for submission is Wednesday 30 June 2010. For further details please visit our website at www.soci.org/events.

## Bursaries

A limited number of student registration bursaries will be available for this event. To apply for a bursary, contact conferences@soci.org. Places are awarded on a first come, first served basis.

## Organisers

Rogier Buijsman, MSD, Netherlands
Rebecca Butler, Novartis, UK
Stephen East, Evotec, UK
Karl Gibson, Pfizer, UK
Tom Heightman, Structural Genomics Consortium, UK
Caroline Low, Imperial College, UK
Jonathan Mason, Lundbeck, DK
Martin Owton, Lilly, UK
Jac Wijkmans, MSD (KNCV Representative), Netherlands

## Information on SCI

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SCI is the publisher of many well respected journals and industry leader Chemistry & Industry magazine (C&I). SCI can offer a network of contacts spanning education, science and business, an in-depth knowledge of chemical related industries together with a rolling programme of conferences, awards and scholarships to help further knowledge and support those involved in the sector no matter what stage of their careers.

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## Venue and Travel

The conference will be held at the MSD site in OSS. The site has been based in Oss since 1923 and its business activities include; research & development (MRL), manufacturing operations API/Biotech and manufacturing operations pharmaceuticals. Site Oss also plays a central role for Women's Health and the Central Nervous System.

### By air

The nearest airport serving Oss is Amsterdam Schiphol Aiport. For further information, visit www.schiphol.nl (available in several languages).

### By train

Trains to Oss from Amsterdam and Schiphol Airport require a change at 's-Hertogenbosch (Den Bosch). There are two trains per hour to Den Bosch from the Airport (journey time 1 hour 10 minutes). There are four trains per hour from Den Bosch to Oss (journey time 10-15 minutes). The same number run from Nijmegen (journey time 15 minutes). Times and prices can be found on the website of Netherlands Railways: www.ns.nl.

The MSD site is very close to the rail station on the line between 's-Hertogenbosch and Nijmegen. Please note that the station is Oss and not Oss West, which is on the same line. The site entrance is on Molenstraat, a few minutes walk from the station.

### By road

For full directions by road, please visit www.soci.org/events.

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**W**: http://www.cityhotel.nl

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